Gauge-Away Effect in Cold Gases on Optical Lattices

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It is shown that a simple modification of the geometry in which Raman lasers are applied to a cold gas in an optical lattice results in transforming the emerging effective electromagnetic field into a pure gauge. This contrived *gauge-away* effect can be observed experimentally by measuring the Mott-Insulator-to-Superfluid critical point. The underlying mechanism for this phenomenon is the ability to engineer the transfer of the transverse component of the gauge potential into its longitudinal one.

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Ultracold gases on optical lattices provide a powerful instrument for creating quantum devices that can simulate, in a controlled manner, a variety of condensed matter systems. The emerging possibility of acting on the system with carefully tuned electromagnetic fields invites the design of a new generation of experiments [1]. In particular, it is in principle possible to implement effective Abelian [2, 3, 4] and non-Abelian [5] gauge fields coupled to the Hubbard model, which describes the physics of an ultracold gas on an optical lattice. For the off-lattice implementations see [6, 7]; for the rotation-based approach see [8]. This would provide a remarkable realization of man-made effective gauge symmetry.

To obtain a clear understanding of effective gauge fields on optical lattices, simple experiments with neat signatures must be devised to prove the purported gauge phenomenon. Note that, in this context, the gauge fields are not real ones, nor are the particles they are coupled to electrically charged particles. The system is just behaving according to a Hamiltonian that simulates an effective, non-dynamic gauge interaction. Therefore, a precise characterization of what the equivalent of gauge effects are must be put forward.

A word of caution, however, is in order. In the cold atom system the expectation value of any hermitian operator, in particular the vector potential, is accessible experimentally. Conversely, in actual gauge systems, be it a quantum Hall sample or quantum chromodynamics, observables must not only be hermitian but they must also be gauge-invariant. Since no real dynamic gauge-symmetry is present in cold atom simulations, the exciting possibility of performing experiments revealing information that would not be accessible in the real world presents itself. For instance, gauge-dependent effective vector fields have been observed in Ref. [9], where a Bose-Einstein condensate subjected to an optically generated effective magnetic field was studied experimentally. The authors reported distinguishing between different zero magnetic field configurations. Also, see the viewpoint [10].

We here propose a scheme to experimentally simulate a very specific gauge property of the interactions that are controlled on an optical lattice. The idea consists in exploiting a simple variation of the geometry of a known experimental setup to 'gauge-away' the effective, non-dynamic Abelian gauge field. That is, while no change is made on the intensity of the lasers acting on the optical lattice, the Abelian electromagnetic potential they effectively generate can be transformed at will from a would-be physical field into a would-be pure gauge, i.e. with zero electric and magnetic field. As a consequence, the measurement of any gauge-invariant observable must reflect the disappearance of the effective gauge field. Thus, a gauge-away effect could be observed by means of a simple angle rotation of external laser fields.

Another way of understanding our proposal is as follows. The effective gauge fields generated in the optical lattices are non-dynamic. The only way to have a gauge transformation is to modify the action of the external lasers. In a way, we can physically perform gauge transformations. We can also modify at will whatever part of a gauge field is longitudinal or transverse and check how this affects observables. The gauge-away effect corresponds to specifying the experimental manipulation that produces a transfer from the transverse to the longitudinal components of a gauge potential.

From a theoretical point of view, our modification of the setup of cold gases on optical lattices coupled to external magnetic fields needs a detailed analysis. We shall first present the basic elements of our proposal so as to describe an experimental signature that would reveal the gauge-away effect. Then, we shall analyze some of the subtleties that appear in the theoretical description of the system due to the change in the configuration of the experiment.

Let us begin our discussion by recalling that cold bosonic atoms propagating on a sufficiently deep optical lattice are adequately described by the single-band Bose-Hubbard model [11, 12]. In recent years, several proposals have been put forth whereby the standard setup for generating an optical lattice in the lab is modified in such a way that the hopping terms in the Hubbard Hamiltonian acquire a position-dependent phase. For an infinite two-dimensional lattice the Hamiltonian reads

$$\begin{aligned} H \;=\; & -J_x \sum_{m,n=-\infty}^{\infty} e^{i\theta^x_{m,n}} a^\dagger_{m+1,n} a_{m,n} + h.c. - \\ & -J_y \sum_{m,n=-\infty}^{\infty} e^{i\theta^y_{m,n}} a^\dagger_{m,n+1} a_{m,n} + h.c. + \\ & +\frac{U}{2} \sum_{m,n=-\infty}^{\infty} N_{m,n}(N_{m,n}-1) - \sum_{m,n=-\infty}^{\infty} \mu_{m,n} N_{m,n}\,, \end{aligned} \tag{1}$$

where $a^\dagger_{m,n}$ and $a_{m,n}$ create and destroy an atom at a lattice site (m,n), respectively, and obey the usual bosonic commutation relations. The constant J_x (J_y) is the site-to-site tunneling energy in the x (y) direction. The parameter U is the

pair interaction energy at each site, $\mu_{m,n}$ is the local chemical potential, and $N_{m,n}$ is the local occupation. Most remarkably, bosons hopping on the lattice acquire position-dependent phases $\theta^x(m,n)$ and $\theta^y(m,n)$.

The previous Hamiltonian closely resembles that of charged particles on a lattice interacting with a classical magnetic field perpendicular to it. As in the case of ordinary charged particles, from Eq. 1 it is clear that bosons traveling around a closed loop pick up a phase shift proportional to the magnetic flux going through the area bounded by the loop. Henceforth, we will identify the phases $\theta^i_{m,n}$, with the components of an effective vector potential $A^{ef}_i(m,n)$, $i = x, y$. Note that $A^{ef}_i(m,n)$ is only an effective non-dynamic description of the system. It is not a fundamental field, it does not propagate, it is not subject to gauge symmetry.

Nevertheless, we can make physical modifications of external lasers that mimic gauge transformations. This permits the following symmetry. The modified Hubbard Hamiltonian is invariant under a local transformation of $A^{ef}_i(m,n)$ and of the creation and destruction operators given by

$$\begin{aligned} A^{ef}_x(m,n) &\to A^{ef}_x(m,n) - (\Lambda(m+1,n) - \Lambda(m,n)), \\ A^{ef}_y(m,n) &\to A^{ef}_y(m,n) - (\Lambda(m,n+1) - \Lambda(m,n)), \\ a_{m,n} &\to e^{i\Lambda(m,n)} a_{m,n}\,, \\ a^\dagger_{m,n} &\to e^{-i\Lambda(m,n)} a^\dagger_{m,n}\,, \end{aligned} \tag{2}$$

for any function $\Lambda(m,n)$, which is vividly reminiscent of a gauge transformation in an ordinary electromagnetic system. Let us stress here that, despite the invariance of the Hamiltonian under Eq. 2, in the cold atom setup the phases $\theta^i_{m,n} = A^{ef}_i(m,n)$, and consequently the effective gauge field, are physical quantities. In order to perform a gauge transformation on the effective vector potential one must alter the configuration of the experimental setup, as the local phases $\theta^i_{m,n} = A^{ef}_i(m,n)$ must be changed. Note that the invariance of the Hamiltonian under Eq. 2 maps the solutions of gauge-equivalent configurations to each other if only gauge-invariant observables are considered. This fact is far from obvious from the point of view of the standard theory of degenerate gases.

Let us now present a way to realize the above modified Hubbard model that allows for an experimental verification of a gauge-away effect. The basic idea remains to change appropriately the action of external laser fields so as to transfer the transverse part of the generated effective gauge field into a longitudinal part. Then, gauge-invariant observables will only depend on the former one.

Of the different ways to create an artificial magnetic field in a two-dimensional non-rotating optical lattice [2, 3, 4], let us focus our attention on the experimental scheme proposed in Ref. [2]. In this setup, atoms in different hyperfine states are trapped in different columns of the lattice by adequately polarizing the standing wave of light that forms it. The hopping in the direction of these columns, x, is unaltered and as usual it is controlled only by the lattice depth in that direction, V_x. The hopping in the other direction, y, is controlled by extra lasers which induce Raman transitions between the two hyperfine states with a complex Rabi frequency. When an atom in a given hyperfine state changes to the other state, it is no longer at a minimum of the lattice potential and is compelled to move to one of the neighboring columns. In order to ensure that the tunneling along y is solely controlled by these additional lasers, the relation $V_x << V_y$ must hold. This allows us to set the non-Raman induced hopping in the y direction, J_y, safely to zero in the same way J_z must be negligible for a two-dimensional optical lattice.

Let $|g\rangle$ and $|e\rangle$ be the two hyperfine levels. The Rabi frequency at the lattice position $\mathbf{x} = (m, n/2)a$ is $\Omega(\mathbf{x}) = \Omega_0 e^{\pm i(\mathbf{k}_e - \mathbf{k}_g)\mathbf{x}}$, where $\mathbf{k}_g$ and $\mathbf{k}_e$ are the wave-vectors of the Raman lasers, Ω_0 is a constant and a is the lattice spacing. As pointed out in the original work, the tunneling amplitude in the y direction is a complex function and is related to the average of the Rabi frequency $\Omega(\mathbf{x})$ with Wannier functions, localized and orthogonal superpositions of Bloch waves, at consecutive sites. Contrary to the original proposal we will not restrict the vector $\mathbf{q} = \mathbf{k}_e - \mathbf{k}_g$ to lie along the x direction. This modification is what allows the hopping phase in the y direction to depend on m as well as on n,

$$A^{ef}_y(m,n) \propto (\mathbf{k}_e - \mathbf{k}_g)\cdot\mathbf{x} = mqa\cos\theta + \underbrace{\frac{n}{2}qa\sin\theta}_{\textbf{pure gauge}}\,, \tag{3}$$

where q is the modulus of $\mathbf{q}$ and θ is the angle between $\mathbf{q}$ and the x-axis of the lattice. The proportionality constant between $A^{ef}_y(m,n)$ and $(\mathbf{k}_e - \mathbf{k}_g)\cdot\mathbf{x}$ will be computed later on. In this setup, the Raman transitions induce no translations in the x-axis direction, hence A^{ef}_x is identically zero for all values of θ and q. Moreover the n-dependence of A^{ef}_y is a pure gauge, i.e. it has no effect on the simulated magnetic field or on any other gauge-invariant observable. That is to say, for $\theta = \pi/2$, we have a non-trivial, position-dependent hopping phase $A^{ef}_y(n) = \frac{n}{2}qa$, while the magnetic field is null,

$$B_z = A^{ef}_y(m+1,n) - A^{ef}_y(m,n) \underset{\theta\to\pi/2}{\longrightarrow} 0\,. \tag{4}$$

Consequently, by rotating the Raman lasers to the special angle $\theta = \pi/2$ the simulated magnetic field B_z is gauged-away and the system is in effect simulating a trivial field in a highly non-trivial way.

From a practical point of view, gauge-invariant observables can be computed in any gauge. Therefore, we are free to shift $A^{ef}_y \to \bar{A}^{ef}_y$ to a more convenient gauge. To be precise, we can work out gauge-invariant observables using the gauge transformation $\Lambda(n) = qa\sin\theta/4n(n-1)$ that removes the n-dependence of A^{ef}_y. Then, for all gauge-invariant computational purposes, the effective Hamiltonian that governs the bosons on the optical lattice is

$$\begin{aligned} H = &-J\sum_{m,n=-\infty}^{\infty}(a^\dagger_{m+1,n}a_{m,n} + e^{i\bar{A}^{ef}_y(m)}a^\dagger_{m,n+1}a_{m,n} + h.c.) + \\ &+\frac{U}{2}\sum_{m,n=-\infty}^{\infty}N_{m,n}(N_{m,n}-1) - \sum_{m,n=-\infty}^{\infty}\mu_{m,n}N_{m,n}\,, \end{aligned} \tag{5}$$

where J is calculated by taking the modulus of the average of $\Omega(\mathbf{x})$ with Wannier functions centered at consecutive sites and now $\bar{A}^{ef}_y(m) = m\alpha\cos\theta$, where $\alpha = \frac{qa}{2\pi}$.

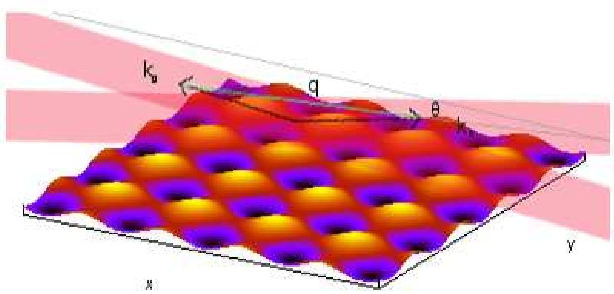

FIG. 1: Diagram depicting the geometry of the configuration. The Raman lasers, with wave vectors $\mathbf{k}_g$ and $\mathbf{k}_e$, are rotated simultaneously with respect to the lattice in such a way that the angle θ between the difference $\mathbf{q} = \mathbf{k_e} - \mathbf{k_g}$ and the x-axis, and thus the effective magnetic flux per plaquette, changes. The pure gauge configuration corresponds to $\theta = \pi/2$, that is, for $\mathbf{q}$ parallel to the y-axis.

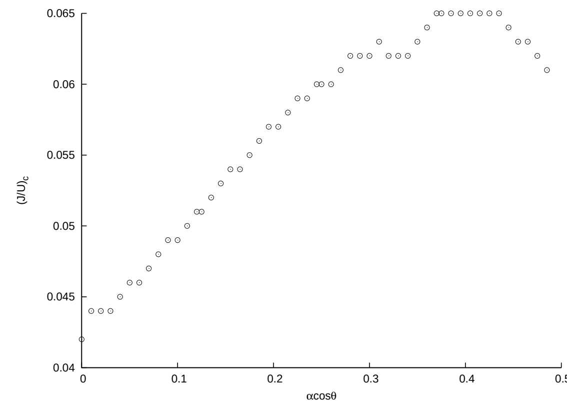

FIG. 2: Critical parameter $(J/U)_c$ as a function of the magnetic flux $\Phi = \alpha \cos\theta$. The phase diagram was determined using the mean field approximation for a 40×40 square lattice with open boundary conditions for $\mu_{m,n} = 0.5$ and with no trap. As the angle of external lasers is changed, the transfer from transverse to longitudinal effective gauge field makes the MI-SF transition to change the location of its critical point. This corresponds to a gauge-away effect of the effective gauge field. For $\alpha\cos\theta \to 0$, the hopping phase is $\theta^y(m,n) = A_y^{ef}(m,n) = \alpha n/2$, and the MI-SF transition point appears at the known value $(J/U)_c = .043$. Although site-dependent phases are present, this transition point remains unchanged because $A_y^{ef}(m,n)$ is completely gauged-away, as it only depends on n. Only the interval $\Phi \in [0, 0.5]$ is considered because the Hamiltonian in Eq. 5 is invariant under the replacement $\Phi \to 1 - \Phi$.

Working with the transformed Hamiltonian, the gauge-away effect can be rephrased. In the configuration $\theta = \pi/2$, i.e. $\bar{A}_y^{ef} = 0$, the system must be oblivious to the fact that the hopping in the y direction carries the original associated phase $\theta^y_{m,n}$. In other words, due to the fact that for this special angle the system is gauge-equivalent to the Bose-Hubbard Hamiltonian with real, constant hopping amplitudes it follows that the actual system in the lab must behave accordingly.

To realize the gauge-away effect experimentally it is first necessary to identify an observable. A natural candidate arises in the context of the Mott insulator (MI) to superfluid (SF) transition, which has been studied extensively both theoretically and experimentally in cold atoms on optical lattices (see Ref. [8] and references therein). The experimental signature of the MI phase is the absence of structure (peaks) in the momentum distribution of the gas, $G(\mathbf{k}) \sim |w(\mathbf{k})|^2 \sum_{\mathbf{R},\mathbf{R'}} e^{ik\cdot(\mathbf{R}-\mathbf{R'})}\langle a^\dagger_{\mathbf{R}} a_{\mathbf{R'}}\rangle$, where $w(\mathbf{k})$ stands for the Wannier function in momentum space. Conversely, in the SF phase the momentum distribution shows pronounced peaks at the momentum values of the reciprocal lattice. This is due to the fact that for the MI phase, $|\langle a^\dagger_{\mathbf{R}} a_{\mathbf{R'}}\rangle| \to 0$, while in the SF phase $|\langle a^\dagger_{\mathbf{R}} a_{\mathbf{R'}}\rangle| \to constant$, for $|\mathbf{R} - \mathbf{R'}| \to \infty$.

A crucial observation is that $|\langle a^\dagger_{\mathbf{R}} a_{\mathbf{R'}}\rangle|$ at large separation acts as a gauge-invariant order parameter for the MI-SF transition. Indeed, $\langle a^\dagger_{\mathbf{R}} a_{\mathbf{R'}}\rangle$ transforms multiplicatively with the phase $e^{i(\Lambda(\mathbf{R})-\Lambda(\mathbf{R'}))}$ and it only vanishes in the SF phase. It follows that the MI-SF phase diagram in the $J/U - \alpha$ plain can serve as a witness to the gauge-away effect.

The exact computation of the order parameter for the MI-SF transition is not possible due to the difficulty of solving the modified Hubbard model exactly for a large lattice. This observable can be approximated by a mean field computation, which is known to reflect the MI-SF phase transition. To compute an approximate ground state of the Hamiltonian in Eq. 5 and determine the critical point at different values of the magnetic flux, we proceed by decoupling the Hilbert spaces of adjacent lattice sites in occupation space by the replacement [13] $a^\dagger_{m+1,n} a_{m,n} \to \psi^*_{m,n} a^\dagger_{m+1,n} + \psi_{m+1,n} a_{m,n} - \psi^*_{m,n}\psi_{m+1,n}$. The quantities $\psi_{m,n}$, computed according to the relation $\psi_{m,n} = \langle a^\dagger_{m+1,n}\rangle$, are variational parameters over which the energy is to be minimized. A random initial set of $\psi_{m,n}$ allows for a diagonalization of the Hamiltonian in the truncated occupation basis. The eigenvector with lowest lying eigenvalue is then used to compute a new set of $\psi_{m,n}$. The process is then repeated recursively and stopped when $\psi_{m,n}$ converges to a fixed point.

The numerical convergence of the iterative mean field method is severely affected by the addition of the effective gauge field. We find many different minimum energy solutions of $\psi_{m,n}$. This is consistent with the fact that the Hamiltonian commutes with the momentum in the y direction and the ground state is degenerate. In addition, for certain values of $\alpha\cos\theta$ and for certain initial conditions the process does not converge, it oscillates between two different non-vanishing values of of $\psi_{m,n}$. Nevertheless, this does not occur in the MI phase, where $\psi_{m,n} = 0$ is the only attractor, so it should not affect the phase diagram appreciably. The results are consistent with those obtained in a perturbation expansion in J [14], and with those obtained by a modified mean field approach in Ref. [15].

The phase diagram we obtain numerically, see Fig. 2, shows an approximately linear dependence of $(J/U)_c$ on $\alpha\cos\theta$ for a range of values of $\cos\theta$. As the total effective magnetic flux per unit plaquette, $\Phi \equiv \alpha\cos\theta$, decreases, the transverse component of the effective vector potential is transferred to its longitudinal component, until it is purely longitudinal for $\cos\theta = 0$. When this particular configuration is

reached the MI-SF transition takes place at the same value of $(J/U)_c$ as it does for the un-modified Hubbard model because it is a gauge-invariant observable that does not depend on the longitudinal part of the vector potential. That is, the position-dependent hopping phase introduced by the Raman lasers $\theta^y(m,n) = \alpha n/2$ has no effect (it is gauged away) because it is identified with the longitudinal component of the the gauge field, $A_y^{ef}(m,n) = \alpha n/2$. In summary, the gauge away effect we present can then be experimentally observed as an increase of the point at which the MI-SF phase transition takes places when the angle of Raman lasers is varied.

Let us now discuss two technical details that have been left apart. First, we need to check that the modified Hubbard model is a good representation of the system and, second, the parameters of the model can be fixed at our convenience. We start by recalling that the matrix element corresponding to the Rabi oscillation between the $|e\rangle$ and $|g\rangle$ states takes the form of an average over Wannier functions [2], $J_y^{ram}(m,n) = \frac{\hbar}{2}\int \mathrm{d}^2\mathbf{x}\,\mathbf{w}^*(\mathbf{x}-\mathbf{x}_{\mathrm{m,n}})\,\Omega\,\mathbf{w}(\mathbf{x}-\mathbf{x}_{\mathrm{m,n+1}})$. Using the fact that the Wannier functions factorize, $\mathbf{w}(\mathbf{x}) = w_x(x)w_y(y)$, it is

$$J_y^{Ram} = \frac{\hbar}{2}\Omega_0 e^{i\tilde{A}_y^{ef}(m,n)}\int \mathrm{d}x'\,|w_{x'}(x')|^2\cos(2\alpha\cos\theta\,x') \times \int \mathrm{d}y' w_{y'}^*(y')\mathrm{e}^{\mathrm{i}(2\alpha\sin\theta\,y')}w_{\mathrm{y}'}(y'-\frac{\pi}{2})\,, \tag{6}$$

where $\tilde{A}_y^{ef} = 2\pi\alpha(\cos\theta\,m + \sin\theta\,n/2)$. The difference between $\tilde{A}_y^{ef}$ and the actual gauge field A_y^{ef} is given by a spatially constant (but θ dependent) phase contribution coming from the integral in the second line and can be omitted.

We are ready to address the first technicality. For Eq. 6 to be a reliable calculation of the Raman-assisted tunnelling it is necessary that Ω_0 be small with respect to the optical potential that forms the lattice. Furthermore, the tilting of the lattice, a crucial ingredient in this construction, must in turn be small compared to the energy gap to the second band and be large compared to Ω_0. A numerical evaluation of $J \equiv |J_y^{Ram}|$ shows all the above relations can be satisfied simultaneously for all θ while meeting the requirement $J = J_x$.

The second technicality is perhaps a more relevant issue. The experimental setup must remain well calibrated for any value of the magnetic flux $0 \leq \Phi \leq 1$. From Eq. 6 $J = J(\alpha,\theta)$, so the ratio J/J_x could significantly vary in Φ. If this were the case the degree of anisotropy in the model would be θ-dependent and could obscure the effects of the effective magnetic field. For different choices of the lattice potentials V_i, $i = x,y,z$ compatible with tight-binding approximation and with the requirement that the free hopping J_y and J_z be suppressed shows that this problem can be avoided by working at fixed α. For instance, in the case $V_{0x} = 16E_R, V_{0y} = 25E_R$, where E_R is the lattice's recoil energy, the maximum variation J in α is more than 25% while the maximum variation J in θ is 4%. Note that the two variations go in opposite directions. It follows that it is possible, at least in principle, to define the curves $\tilde{\alpha}(\Phi)$ and $\tilde{\theta}(\Phi)$ such that J remain precisely constant, $J(\tilde{\alpha}(\Phi),\tilde{\theta}(\Phi)) = J_x$, $0 \leq \Phi \leq 1$.

The following experimental procedure could be used in order to minimize the deviation of J/J_x from unity. Once suitable values of the V_i have been chosen, we start with a pure gauge configuration (i.e. $\theta = \pi/2$). To maximize α, we fix the relative angle of the lasers to π. At this point, we can perform diffusion experiments as in [12] for different Rabi frequencies Ω_0 (whose value is controlled by the frequencies of the Raman lasers). By determining the value of Ω_0 for which diffusion rates in the x and y directions become equal, we can, at the same time, check that the pure gauge configuration corresponds to the free hopping model with $J(\theta = \pi/2) = J^x$ and prepare the system for the addition of the effective external magnetic field. Indeed, to turn on B_z we only need to change the angle θ from $\pi/2$ without modifying any of the other parameters.

In conclusion, we have shown that the Hubbard Hamiltonian with position-dependent complex hopping phases serves as a laboratory to create man-made effective gauge transformations. It is then possible to devise a gauge-away experiment, based on the idea of transferring all the transverse part of the effective gauge potential to its longitudinal one, only by modifying the angle between the Raman laser fields and the optical lattice. Thus, a gauge-invariant observable such as the critical value $(J/U)_c$ for the MI-SF phase transition point changes in a predictable manner as the effective vector potential is gauged away.

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